14	CAS No.: 606-20-2	Substance: 2,6-Dinitrotoluene

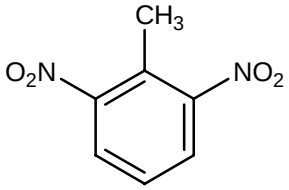
Chemical Substances Control Law Reference No.: 3-446 (as dinitrotoluene)

PRTR Law Cabinet Order No.: 1-157 (as dinitrotoluene)

Molecular Formula: $C_7H_6N_2O_4$

Molecular Weight: 182.14

Structural Formula:



1. General information

The aqueous solubility of this substance is 182 mg/L (20°C) and the partition coefficient (1-octanol / water) (log Kow) is 2.10. The vapor pressure is 2.87×10^{-4} mmHg (= 0.0383 Pa) (20°C). Degradability (aerobic degradation) in terms of BOD-based degradation percentage is estimated to be 0 %, and the bioconcentration of this substance is thought to be zero or very low. In addition, this substance does not have hydrolyzable groups.

Dinitrotoluene is a Type 2 and Type 3 Monitoring Chemical Substance under the Law Concerning the Examination and Regulation of Manufacture, etc. of Chemical Substances and a Class 1 Designated Chemical Substance under the Law concerning Reporting, etc. of Releases to the Environment of Specific Chemical Substances and Promoting Improvements in Their Management (PRTR Law). It is used primarily as organic syntheses, a raw material of toluizine, dyes, and an intermediate compound of explosive. The quantity of production and import in FY2004 was 195 tons. The contents of Dinitrotoluene isomers in the general chemical products were approximately 75% for 2,4-Dinitrotoluene and approximately 20% for 2,6-Dinitrotoluene.

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2. Exposure assessment

Total release of Dinitrotoluene to the environment in FY2004 under the PRTR Law came to approximately 0.68 tons, all of which was reported. Release to the public water bodies accounted for a large part of the reported release. Chemical Industry accounted for all of the reported release.

The distribution into each environment medium predicted by means of a multimedia model was 86.3% for water bodies and 10.3% for bottom in the case of the region where the release quantity to the environment and public water bodies was considered to be the maximum. In the case of the region where the release quantity to the atmosphere was considered to be the maximum, the distribution was 85.5% for water bodies and 10.2% for bottom.

The predicted maximum exposure concentration for inhalation exposure to human beings was approximately 0.0086 μg/m^3. The predicted maximum oral exposure was estimated to be less than 0.0204 μg/kg/day.

The predicted environmental concentration (PEC) that indicates exposure to aquatic organisms was estimated to be 0.06 μg/L for freshwater and less than 0.01 μg/L for seawater public water bodies.

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3. Initial assessment of health risk

This substance may have effects on blood and may produce methemoglobin. The inhalation or ingestion may result in blue lips, nails and skin, headache, dizziness, nausea, confusion, convulsion, and unconsciousness. Contact with the skin may be absorbed and cause the similar symptoms.

There was insufficient information regarding the carcinogenicity of the substance. For this reason, an initial assessment of the substance was conducted based on information of non-carcinogenic effects.

As the ‘Non-toxic level’ for the oral exposure, the LOAEL of 4 mg/kg/day (extramedullary hematopoiesis) was obtained from the medium- and long-term toxicity testing in dogs. As this is a LOAEL, it was divided by 10, and because of short experimental period, the value was further divided by 10, and a value of 0.04 mg/kg/day as the ‘Non-toxic level’. For inhalation exposure, the

'Non-toxic level' could not be estimated.

With regard to oral exposure, in case of intakes of the groundwater and food, the predicted maximum exposure was approximately less than 0.02 μg/kg/day. The MOE of exceeding 40 was derived from the 'Non-toxic level' of 0.04 mg/kg/day divided by the predicted maximum dose, and divided by 10, because the 'Non-toxic level' was established by means of animal testing, and considering the carcinogenesis, it was further divided by 5. Accordingly, its health risk for oral exposure to this substance could not be identified. One of the causes may be the detection limit being relatively high. However, the exposure to this substance through food intakes are assumed to be low, and there would be low necessity of giving priority to the obtaining of the exposure amount by lowering the detection limit .

For the inhalation, because its 'Non-toxic level' was not determined, its health risk could not be identified. Release to the atmosphere of this substance accounted for only 7% in the total release of Dinitrotoluene (reported quantity of release: 0.68 tons) and it is expected that almost all of it is distributed into the mediums other than the atmosphere. As a reference, assuming that the absorption rate is 100 %, and the 'Non-toxic level' for the oral exposure is converted to the 'Non-toxic level' for the inhalation, the value is 0.13 mg/m^3. The MOE determined from this figure and the predicted maximum exposure concentration is 300. Accordingly, there would be relatively low necessity of collecting information on inhalation exposure to this substance in the ambient air for its health risk assessment at present.

Information of toxicity				Exposure assessment		Result of risk assessment			Judgment
Exposure path	Criteria for risk assessment	Animal	Criteria for diagnoses (endpoint)	Exposure medium	Predicted maximum exposure quantity and concentration				
Oral	'Non toxic level' 0.04 mg/kg/day	Dogs	extramedullary hematopoiesis	Drinking water, food	– μg/kg/day	MOE	–	×	×
				Groundwater , food	< 0.02 μg/kg/day	MOE	> 40	×	
Inhalation	'Non toxic level' – mg/m^3	–	–	Ambient air	0.0086 μg/m^3	MOE	–	×	×
				Indoor air	– μg/m^3	MOE	–	×	×

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4. Initial assessment of ecological risk

With regard to acute toxicity, reliable information of a 72-hour EC_{50} growth inhibition value of 15,000 μg/L was found for the algae *Pseudokirchneriella subcapitata*, a 48-hour EC_{50} immobilization value of 20,300 μg/L was found for the crustacea *Daphnia magna* (water flea), and a 96-hour LC_{50} value of 18,500 μg/L was found for the fish *Pimephales promelas* (fathead minnow). Accordingly, an assessment factor of 100 was used, a predicted no effect concentration (PNEC) of 150 μg/L was obtained based on the acute toxicity values. With regard to chronic toxicity, reliable information of a 72-hour no observed effect concentration (NOEC) growth inhibition value of 5,000 μg/L was found for the algae *P. subcapitata*, and a 21-day NOEC reproduction value of 60 μg/L was found for the crustacea *D. magna*. As the PNEC for the substance, a value of 0.60 μg/L obtained from the chronic toxicity for the crustacea was used.

The PEC/PNEC ratio was 0.1 for freshwater bodies and less than 0.02 for seawater bodies. Accordingly, efforts to gather information are thought to be required. There is thought to be need to examine improvement of the information of ecological toxicity, understanding production and import quantities and changes etc. of release and transfer quantities under the PRTR Law.

Hazard assessment (basis for PNEC)			Assessment factor	Predicted no effect concentration PNEC (μg/L)	Exposure assessment		PEC/ PNEC ratio	Result of assessment
Species	Acute / chronic	Endpoint			Water body	Predicted environmental concentration PEC (μg/L)		
Crustacea (water flea)	Chronic	NOEC reproduction	100	0.60	Freshwater	0.06	0.1	▲
					Seawater	< 0.01	< 0.02	

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5. Conclusions

	Conclusions		Judgment
Health risk	Oral exposure	Impossible of risk characterization. It is thought to be little need to give priority to understanding the exposure amount after lowering the lowest limit of detection.	×
	Inhalation exposure	Impossible of risk characterization. However, there is thought to be comparatively little need to collect information, etc.	×
Ecological risk	Requiring information collection. There is thought to be need to examine improvement of the information of ecological toxicity, understanding production and import quantities and changes etc. of release and transfer quantities under the PRTR Law.		▲

［Risk judgments］ ○: No need of further work ▲: Requiring information collection
■: Candidates for further work ×: Impossible of risk characterization

Non-toxic level *

・When a LOAEL is available, it is divided by 10 to obtain a level equivalent to NOAEL.

・When an adverse effect level for the short-term exposure is available, it is divided by 10 to obtain a level equivalent to an adverse effect level for the long-term exposure.